Conductivity in wide-bandgap oxides: overcoming electron localization

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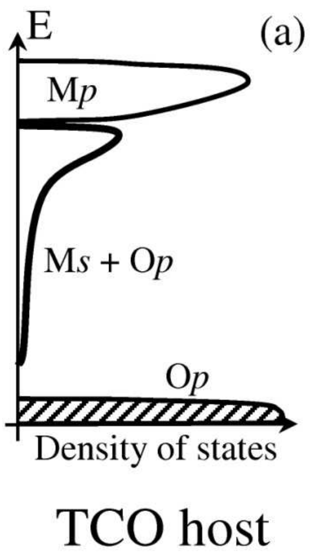
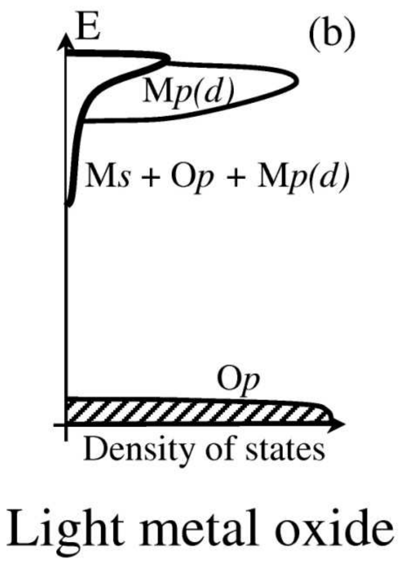
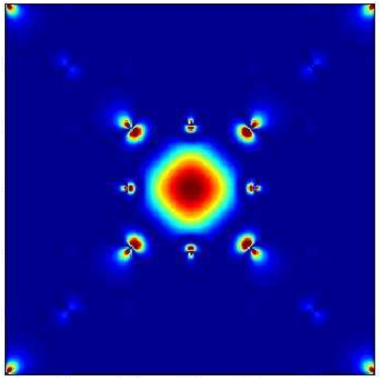
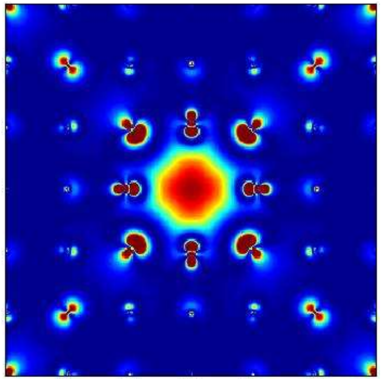
Main group metal oxides such as MgO, CaO, Al_2O_3, ZnO and In_2O_3, share the same electronic configuration of cations, yet, their electrical properties are very different – the first three are classical insulators while the oxides of post-transition metals can be easily converted into metallic conductors.







Electron localization near oxygen vacancy site (F-center) in MgO



Vacancy-induced electron charge density spreads throughout ZnO crystal, a transparent conductor

Our comparative electronic band structure studies reveal that the proximity of the cation's empty p-states to the conduction band bottom plays the key role in determining the transport properties of oxygen deficient materials.

Results for conductive $Ca_{12}Al_{14}O_{33}$ suggest a way to overcome the electron localization and efficiently utilize the abundant, environmentally-friendly magnesia, lime and alumina as complex transparent conducting oxides.